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#### PASSWORD:

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FULL ESTIMATED COST	ENTRY 102.95	SESSION 564.39
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-14.82	-28.08
=> file registry COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE	-14.82	-28.08

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Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1 DICTIONARY FILE UPDATES: 18 SEP 2007 HIGHEST RN 947490-11-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

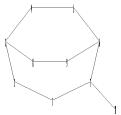
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10573132\10573132a.str





chain nodes :

10

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-10

ring bonds :

 $1-2 \quad 1-7 \quad 2-3 \quad 3-4 \quad 3-8 \quad 4-5 \quad 5-6 \quad 6-7 \quad 6-9 \quad 8-9$ 

exact/norm bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 6-9 8-9

exact bonds :

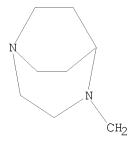
7-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

## L10 STRUCTURE UPLOADED

=> d 110 L10 HAS NO ANSWERS L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 110

SAMPLE SEARCH INITIATED 17:50:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3760 TO ITERATE

53.2% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 71523 TO 78877 PROJECTED ANSWERS: 2 TO 191

2 ANSWERS

L11 2 SEA SSS SAM L10

=> d scan

```
L11 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 4-Aza-1-azoniabicyclo[3.2.2]nonane, 4-hexyl-6-(hydroxyimino)-3-oxo-1-[[4-[[13-oxo-3-(2-propenyloxy)propyl]amino]carbonyl]phenyl]methyl]-, salt with trifluoroacetic acid (1:1) (9CI)

MF C27 H39 N4 O5 . C2 F3 O2

CM 1

C-NH-CH<sub>2</sub>-CH<sub>2</sub>-C-O-CH<sub>2</sub>-CH-CH<sub>2</sub>

CH<sub>2</sub>

CH<sub>2</sub>

CH<sub>2</sub>

CH<sub>2</sub>

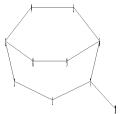
CM 2
```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

 $\label{thm:local-condition} \mbox{ C:\Program Files\Stnexp\Queries\10 series\10573132\10573132b.str}$ 





chain nodes :

10

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-10

ring bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 6-9 8-9

exact/norm bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 6-9 8-9

exact bonds :

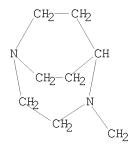
7-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

# L12 STRUCTURE UPLOADED

=> d 112 L12 HAS NO ANSWERS L12 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 112

SAMPLE SEARCH INITIATED 17:51:59 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 3760 TO ITERATE

1 ANSWERS 53.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

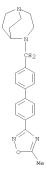
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\* 71523 TO 78877 1 TO 119 PROJECTED ITERATIONS:

PROJECTED ANSWERS:

L13 1 SEA SSS SAM L12

=> d scan

L13 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN IN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4'-(5-methyl-1,2,4-oxadiazol-3-y1)[1,1'-biphenyl]-4-y1]methyl]MF C23 H26 N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 112 full

FULL SEARCH INITIATED 17:52:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 76206 TO ITERATE

65 ANSWERS

100.0% PROCESSED 76206 ITERATIONS

SEARCH TIME: 00.00.02

L14 65 SEA SSS FUL L12

=> d scan

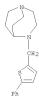
L14 65 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-bromo-2-thienyl)methyl]- (9CI)
MF C12 H17 Br N2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L14 65 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-thienyl)methyl]- (9CI)
MF C18 H22 N2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 173.45 738.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY CA SUBSCRIBER PRICE 0.00 -28.08

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FILE COVERS 1907 - 19 Sep 2007 VOL 147 ISS 13 FILE LAST UPDATED: 18 Sep 2007 (20070918/ED)

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http://www.cas.org/infopolicy.html

=> s 114 9 L14 L15

=> d l15 1-9 ibib abs hitstr

L15 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2006:76714 CAPLUS 2006:76714 CAPLUS 144:150370 144:150370
[1,2,4]Oxadiazol-3-ylbiphenylmethylamines as histamine-3 receptor antagonists and their preparation, pharmaceutical compositions, and use in the treatment of disorders or conditions that may be treated by antagonizing histamine-3 receptors Wager, Travis T.; Howard, Harry R. Pfizer Inc., USA U.S. Pat. Appl. Publ., 23 pp. CODEN: USXXCO DOCUMENT NUMBER: TITLE: INVENTOR (S) . PATENT ASSIGNEE(S): DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE

PATENT NO. KIND DATE APPLICATION NO. DATE

US 2006019998 A1 20060120 US 2005-180185 20050713
CA 2573920 A1 20060202 CA 2005-2573920 20050711
W1 246, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, GE, ES, FI, GB, GD, NN, NN, MN, MX, NX, NX, NI, NN, NN, NX, CM, NN, NN, NN, NX, CM, NS, LS, SM, SY, JJ, TM, TN, TR, TT, ZZ, UA, UG, UZ, VC, VN, VV, ZA, ZM, ZW

RN: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PI, FT, RO, SC, SD, SB, SG, SK, GM, KE, LS, MW, MZ, NA, SD, SL, SS, TZ, SW, TZ, SM, CF, CG, CI, CM, GA, GN, GC, GM, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 1771449 A1 20070411
EP 1771449 A1 20070411
EP 1771A49 A1 20070411
EP 2005-755132 20050711
EP 2004-598933P P 20040721

WO 2005-IB2186 W 20050711

MARPAT 144:150370 OTHER SOURCE(S):

L15 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) arylsulfonyl, or 5- to 10-membered heteroaryl; R3 is (un)substituted C1-8 alkyl, C3-7 cycloalkyl, or C6-14 aryl; or NR1R2 or NR1R3 forms a 4- to 7-membered ring wherein one of the carbons in the ring may be optionally replaced by O, S, NR6, CO, or the ring may be fused to (un)substituted C6-10 arylene, where R6 is H, (un)substituted C1-8 alkyl, 5- to 10-membered (un)substituted (thetero)aryl, or C1-4 alkylcarbonyl; R4 is H or (un)substituted C1-8 alkyl; R5 is H, (F-substituted) C1-6 alkyl, or (F-substituted) C1-6 alkoxy; or pharmaceutically acceptable salts

(P-substituted) C1-6 alkoxy; or pharmaceutically acceptable salts thereof, are claimed in this invention. Example compd. II were prepd. by condensation of 4-bromobenzonitrile with hydroxylamine to give the corresponding N-hydroxyamidine which underwent cyclization with acetic anhydride and the resulting 3-(4-bromophenyl)-5-methyl-[1,2,4]oxadiazole intermediate was coupled with 4-formylphenylboronic acid, to give the oxadiazolylbiphenylcarboxaldehyde, which underwent reductive amination to give example compd. II. An addnl. 71 example compds. use prepd. by this procedure. An assay for detn. of the in vivo affinity of the invention compds. at histanine H3 receptor is described. The percent inhibition of specific binding can be detd. for each dose of the compds., and an IC50 and K1 can be calcd. from these results (no data).

IT 873933-30-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

8/3933-30-39 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses

ses)
(drug candidate; preparation of oxadiazolylbiphenylmethylamines as H3 receptor antagonists for treatment of associated disorders or

conditions RN 87393-30-3 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4'-(5-methyl-1,2,4-oxadiazol-3-y1)[1,1'-biphenyl]-4-y1]methyl]- (CA INDEX NAME)

L15 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

This invention is directed to a class of compds. of formula I as defined herein, or a pharmaceutically acceptable salt thereof; a pharmaceutical composition containing a compound of formula I, a method for treatment AB

of a disorder
or condition that may be treated by antagonizing histamine H3 receptors,
or a method comprising administering to a mammal in need of such
treatment, a compound of formula I, for treatment of a disorder or condition

tion
selected from the group consisting of depression, mood disorders,
schizophrenia, anxiety disorders, Alzheimer's disease, attention-deficit
disorder (ADD), attention-deficit hyperactivity disorder (ADHD),

disorders, sleep disorders, obesity, dizziness, epilepsy, motion sickness.

ress, respiratory diseases, allergy, allergy-induced airway responses, allergic rhinitis, nasal congestion, allergic congestion, congestion, hypotension, cardiovascular disease, diseases of the GI tract, hyper- and hypomotility and acidic secretion of the gastro-intestinal tract. Compds. of formula

where m and n are independently 1, 2 or 3; Xm and Xn are independently B, F, Cl, Br, I, (F-substituted) Cl-6 alkyl, (F-substituted) Cl-6 alkoxy, (un)substituted (Cl-6alkyl)SOp, where p is 0, 1 or 2; R1 and R2 are independently B, (un)substituted Cl-8 alkyl, C3-7 cycloalkyl, C6-14 aryl, (un)substituted 3- at 0.8-membered heterocycloalkyl, (un)substituted C6-10

L15 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) L15 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:1241229 CAPLUS LANGE TEXTS

144:6818

144:6818

1,2-benzoiscs, benzothiazoles, 1,2-benzoisoxazoles, 1,2-benzoisoxhiazoles, and chromones as 67

nicotinic receptor agonists, their preparation, pharmaceutical compositions, and use in therapy Kie, Wenge; Herbert, Brian; Schumacher, Richard A.; Ma, Jianquo; Nguyen, Truc Minh; Gauss, Carla Maria; Tehim, Ashok

Memory Pharmaceuticals Corporation, USA

PCT Int. Appl., 143 pp.

CODEN: PIXXD2

Patent

English

1 DOCUMENT NUMBER: TITLE: INVENTOR(S): PATENT ASSIGNEE(S): DOCUMENT TYPE:

DOCUMENT TIPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE AU 2005-243147 CA 2005-2565984 US 2005-123219 EP 2005-747486 CA 2565984 US 2005272735 EP 1745046 CA 20051984 A1 20051124 CA 2005-2563984 20050506
EP 1745046 A2 20070124 EP 2005-747486 20050506
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
HR, LV, MK, YU
IN 2006DW06854 A 20070831 IN 2006-DN6854 20061117 NO 2006005622 KR 2007015607 PRIORITY APPLN. INFO.: NO 2006-5622 KR 2006-725685 US 2004-568696P 20070202 20061206 20070205 20061206 P 20040507 US 2004-574712P P 20040527 IIS 2004-626469P P 20041110 WO 2005-US15937 W 20050506 US 2005-568696P P 20050507

CASREACT 144:6818; MARPAT 144:6818

ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) underwent oxidative cleavage resulting in the formation of benzoisothiazolecarboxamide IV. Alk. hydrolysis of IV to the carboxylic acid was followed by coupling with 1,4-diazabicyclo[3.2.2]nonane to give compd. V. The preferred compds. of the invention express binding affinities of 5 nM to 2.5 µM (no data).

869783-40-4P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-6-(methoxy)-4H-chromen-4-one 869783-41-5P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-5-(methoxy)-4H-chromen-4-one formate 869783-44-8P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-5-(methoxy)-4H-chromen-4-one formate 869783-44-8P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-7-(methoxy)-4H-chromen-4-one 869783-49-3P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-7-(methoxy)-4H-chromen-4-one 869783-49-3P, 3-(1,4-Diazabicyclo[3.2.2]non-4-ylmethyl)-7-(methoxy)-4H-chromen-4-one formate RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USea) (Uses) (drug candidate; preparation of heteroaryl-substituted diazabicyclo[3.2.2]nonanes as α7 nicotinic receptor agonists)
RN 869783-40-4 CAPLUS
CN 4H-1-Benzopyran-4-one,
3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-6-methoxy(CA INDEX NAME)

OTHER SOURCE(S):

869783-41-5 CAPLUS Formic acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-6-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CM 1 CRN 869783-40-4 CMF C18 H22 N2 O3

64-18-6 C H2 O2

L15 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

The invention relates to heteroaryl-substituted azabicyclic compds.,

, I or II, which are ligands for nicotinic acetylcholine receptors (nAChR) and can be used for the activation of nAChRs and the treatment of disease conditions associated with defective or malfunctioning nicotinic acetylcholine receptors, especially of the brain. In compds. I and II,

CH2, C=0, or C=S; m is 1 or 2; Y is 0 or S; X1 to X4 are independently selected from N and (un)substituted C, wherein at most one of X1 to X4 is N; X5 and X6 are independently selected from CH, fluoro-substituted C1-6 alkoxy-C, and heterocycly1-C, wherein no more than one of X5 and X6 is

X7 is CH or N; and R is H, (halo)-C1-4 alkyl, C3-7 cycloalkyl, C4-7 cycloalkylalkyl, and C1-6 alkyl-C6-10 aryl. The invention also relates

the preparation of the heteroaryl-substituted diazabicyclic compds., pharmaceutical compns. comprising those compds. and a pharmaceutically acceptable carrier, as well as to the use of the compns. as agonists for the  $\alpha^7$  nAchR subtype. Acylation of 3-methoxythiophenol with oxalyl chloride followed by cyclization gave benzothiophenedione III, which

L15 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

о=сн−он

RN 869783-44-8 CAPLUS CN 4H-1-Benzopyran-4-one, 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-5-methoxy-(CA INDEX NAME)

869783-45-9 CAPLUS
Formic acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethy1)-5-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CRN 869783-44-8 CMF C18 H22 N2 O3

CM 2

CRN 64-18-6 CMF C H2 O2

о=сн−он

RN 869783-48-2 CAPLUS CN 4H-1-Benzopytan-4-one, 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-7-methoxy-(CA INDEX NAME)

L15 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

869783-49-3 CAPLUS Despise acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-7-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CRN 869783-48-2 CMF C18 H22 N2 O3

CM

CRN 64-18-6 CMF C H2 O2

о—сн−он

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
thiazolyl, oxazolyl, or imidazolyl, etc.; D is H, alkyl, Ph, or pyridyl,
etc.], useful as nicotinic acetylcholine agonists. For instance,
diazabicyclononane deriv. I was prepd. via reductive amination of
phenylpropargyl aldehyde by 1,4-diazabicyclo[3.2.2]nonane
dihydrochloride.

Biol. investigation included assays for detg. affinity at \( \alpha \) ACDR
and \( \alpha \) ACDR (Ki values were less than 1000 nM in both tests).

IT 849430-68-8P, (1,4-Diazabicyclo[3.2.2]non-4-yl)(6-bromopyridin-2yl)methane
RL: PAC (Pharmacological activity); RCT (Reactant); SFN (Synthetic
preparation); THU (Theraputic use); BTOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of diazabicyclononane derivs. useful as nicotinic
acetylcholine
agonists)
RN 849430-68-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(6-bromo-2-pyridinyl)methyl]- (9CI)

849430-59-7P 849430-60-0P, (1,4-Diazabicyclo[3.2.2]non-4y1) (5-phenylfuran-2-y1)methane 849430-61-1P,
(1,4-Diazabicyclo[3.2.2]non-4-y1) (biphenyl-4-y1)methane
849430-62-2P, (1,4-Diazabicyclo[3.2.2]non-4-y1) (5-phenylthiophen-2y1)methane 849430-63-3P, (1,4-Diazabicyclo[3.2.2]non-4-y1) (benzofuran-2-y1)methane 849430-63-64-PP, (1,4-Diazabicyclo[3.2.2]non-4-y1)
Hazabicyclo[3.2.2]non-4-y1) (haphthalen-2-y1)methane 849430-65-5P,
(1,4-Diazabicyclo[3.2.2]non-4-y1) (1-phenylpropene 849430-66-6P,
(1,4-Diazabicyclo[3.2.2]non-4-y1) (1-phenylpropene 849430-66-6P,
y1/(4,4-Diazabicyclo[3.2.2]non-4-y1) (4-Diazabicyclo[3.2.2]non-4-y1) (quinolin-3-y1)methane 849430-70-2P, (1,4-Diazabicyclo[3.2.2]non-4-y1) (quinolin-2-y1)methane 849430-71-3P,
4-(4-Phenylthiophen-2-y1methyl)-1,4-diazabicyclo[3.2.2]nonane
849430-72-4P, 4-[5-(Pyridin-2-y1)thiophen-2-y1methyl)-1,4-diazabicyclo[3.2.2]nonane 849430-73-5P, 4-(Pyridin-2-y1)methyl)-1,4-diazabicyclo[3.2.2]nonane 849430-73-6P, 4-(Pyridin-2-y1methyl)-1,4-diazabicyclo[3.2.2]nonane
849430-73-PP, 4-(2-Phenylpropyl)-1,4-diazabicyclo[3.2.2]nonane
849430-73-PP, 4-(2-Benzyloxyethyl)-1,4-diazabicyclo[3.2.2]nonane
849430-73-PP, 4-(2-Benzyloxyethyl)-1,4-diazabicyclo[3.2.2]nonane
849430-73-PP, 4-(4-Benzyloxyethyl)-1,4-diazabicyclo[3.2.2]nonane
849430-73-PP, 4-(4-Benzyloxyethyl)-1,4-diazabicyclo[3.2.2]nonane

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:300453 CAPLUS DOCUMENT NUMBER: 142:373869

TITLE:

142:773869
A preparation of diazabicyclononane derivatives,
useful as nicotinic acetylcholine agonists
Ernst, Glen; Phillips, Elfion; Schmiesing, Richard J.
Astrazeneca AB, Swed.; Astrazeneca UK Ltd.
PCT Int. Appl., 34 pp.
CODEN: FIXXD2 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

	PATENT NO.																	
										WO 2004-GB4130								
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BE	, BG	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ	, EC	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS	, JP	KE,	KG,	KP,	KR,	KZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG	, MK	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU	, SC	SD,	SE,	SG,	SK,	SL,	SY,	
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US	, UZ	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SI	, SL	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	ΑT	, BE	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	II	, LU	MC,	NL,	PL,	PT,	RO,	SE,	
		SI,	SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM.	1, GA	GN,	GQ,	GW,	ML,	MR,	NE,	
		SN,	TD,	TG														
					A1 20060628			EP 2004-768673						20040924				
EP	1673	372			В1		2007	0530										
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	JP 2007506723									-5274								
	AT 363484																	
	US 2007043031				2007	0222												
RIORIT:	IORITY APPLN. INFO.:								US	2003	-5066	64P	1	P 2	0030	926		
										WO.	2004	-GB41	30	1	W 2	0040	924	

CASREACT 142:373869; MARPAT 142:373869 OTHER SOURCE(S):

The invention relates to a preparation of diazabicyclononane derivs. of

Q-E-D [wherein: Q is diazabicyclononane derivative; E is alk(en/yn)yl,

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) diazabicyclo[3.2.2]nonane 849430-80-4P 849430-81-5P 849430-82-6P 849430-83-7P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [5:(3-pyridyl)thiophen-2-yl]methane 849430-80-6P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [6:(4-pyridyl)thiophen-2-yl]methane 849430-86-0P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [4-(2-pyridyl)thiophen-2-yl]methane 849430-86-0P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [4-(2-pyridyl)thiophen-2-yl]methane 849430-86-0P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [4-(3-pyridyl)thiophen-2-yl]methane 849430-88-2P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [4-(3-pyridyl)thiophen-2-yl]methane 849430-89-3P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [4-phenylpyridin-2-yl]methane 849430-90-6P, (1,4-Diazabicyclo[3.2.2]non-4-yl) [5-phenylpyridin-2-yl]methane 849430-91-P, 4-(4-Enothiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(5-Enothiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(4-Methoxyphenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(4-Methoxyphenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(5-(4-Chlorophenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-97-9P, 4-(5-(4-Chlorophenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-97-9P, 4-(5-(4-Chlorophenyl)thiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(5-(3-Chlorophenyl)thiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(5-(3-Chlorophenyl)thiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-(5-(3-Chlorophenyl)thiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-05-1P, 4-(7-phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-05-1P, 4-(7-phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-06-P, 4-(2-phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-06-P, 4-(1-methylbenzimidazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-06-P, 4-(1-methylbenzimidazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-06-P, 4-(1-methylbenzimidazol-5-ylmethyl (prepn. of diazabicyclononane derivs. useful as nicotinic acetylcholine agonists)
RN 849430-59-7 CAPLUS

043430-39-7 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(3-phenyl-2-propynyl)- (9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

849430-60-0 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-furanyl)methyl]- (9CI) (CA INDEX NAME)



849430-61-1 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-([1,1'-biphenyl]-4-ylmethyl)- (9CI) (CA INDEX NAME)

RN 849430-62-2 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-thienyl)methyl]- (9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



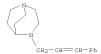
849430-63-3 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-benzofuranylmethyl)- (9CI) (CA INDEX NAME)

849430-64-4 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-naphthalenylmethyl)- (9CI) (CA INDEX NAME)

849430-65-5 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-(3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME) CN

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



849430-66-6 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(benzo[b]thien-3-ylmethyl)- (9CI) (CA INDEX NAME)

849430-67-7 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(2-pyridinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

849430-69-9 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(3-quinolinylmethyl)- (9CI) (CA INDEX NAME)

Page 14

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 849430-70-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-quinolinylmethyl)- (9CI) (CA INDEX NAME)

849430-71-3 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-phenyl-2-thienyl)methyl]- (9CI) (CA INDEX NAME)

849430-72-4 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(2-pyridinyl)-2-thienyl]methyl]-(9CI) (CA INDEX NAME)



849430-73-5 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-([1,1'-biphenyl]-3-ylmethyl)- (9CI) (CA

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) INDEX NAME)



849430-74-6 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



849430-76-8 CAPLUS 1,4-Dlazabicyclo[3.2.2]nonane, 4-[(6-phenyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



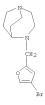
849430-77-9 CAPLUS
1,4-Diazabicyclo[3.2.2]nonane, 4-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

849430-78-0 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)

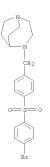
849430-79-1 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-bromo-2-furany1)methy1]- (9CI) (CA INDEX NAME)

(Continued)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

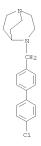


RN 849430-80-4 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane,
4-[[4-[(4-bromophenyl)sulfonyl]phenyl]methy
1]- (9C1) (CA INDEX NAME)

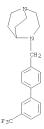


849430-81-5 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4'-chloro[1,1'-bipheny1]-4-y1)methy1]-(9C1) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN



849430-82-6 CAPLUS 1,4-plazabicyclo[3.2.2]nonane, 4-[[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]- (9C1) (CA INDEX NAME)



849430-83-7 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(3-pyridinyl)-2-thienyl]methyl]-(9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH2

RN 849430-84-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(4-pyridinyl)-2-thienyl]methyl](9CI) (CA INDEX NAME)



RN 849430-85-9 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(2-pyridinyl)-2-thienyl]methyl](9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 849430-86-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(3-pyridinyl)-2-thienyl]methyl](9CI) (CA INDEX NAME)



RN 849430-87-1 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-pyridinyl)-2-thienyl]methyl](9C1) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



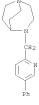
RN 849430-88-2 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(3-isoquinolinylmethyl)- (9CI) (CA INDEX NAME)

RN 849430-89-3 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-phenyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

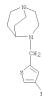


RN 849430-90-6 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-pyridinyl)methyl]- (9CI)
(CA INDEX NAME)

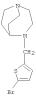
L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 849430-91-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-bromo-2-thienyl)methyl]- (9CI) (CA INDEX NAME)



RN 849430-92-8 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-bromo-2-thienyl)methyl]- (9CI) (CA INDEX NAME)

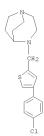


RN 849430-93-9 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-methoxyphenyl)-2-thienyl]methyl]-

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (9CI) (CA INDEX NAME) (Continued)



849430-94-0 CAPLUS
1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-chlorophenyl)-2-thienyl]methyl]-(9CI) (CA INDEX NAME)



849430-95-1 CAPLUS 1,4-biazabicyclo[3.2.2]nonane, 4-[[5-(4-methoxyphenyl)-2-thienyl]methyl]-(9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



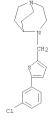
849430-96-2 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(4-chloropheny1)-2-thieny1]methy1]-(9CI) (CA INDEX NAME)



849430-97-3 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(3-chloropheny1)-2-thieny1]methy1]-(9C1) (CA INDEX NAME)

(Continued)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



849430-98-4 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-quinoxalinylmethyl)- (9CI) (CA INDEX NAME)

849430-99-5 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-bromo-5-thiazoly1)methy1]- (9CI)

INDEX NAME)

849431-00-1 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(5-thiazolylmethyl)- (9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN



849431-01-2 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-5-thiazolyl)methyl]- (9CI) (CA INDEX NAME)



849431-02-3 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-1H-imidazol-4-yl)methyl]-(9CI) (CA INDEX NAME)



849431-03-4 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-thiazolylmethyl)- (9CI) (CA INDEX NAME)

Page 17

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

N CH2

RN 849431-04-5 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-benzothiazolylmethyl)- (9CI) (CA INDEX NAME)

S CH<sub>2</sub> N

RN 849431-05-6 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(1-methyl-1H-benzimidazol-2-yl)methyl](9CI) (CA INDEX NAME)

N CH2 N Me

RN 849431-06-7 CAPLUS
CN 1,4-biazabicyclo[3.2.2]nonane, 4-[(3-methyl-5-phenyl-2-thienyl)methyl]-(9Cl) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Me S

RN 849431-07-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-4-thiazolyl)methyl]- (9CI)
(CA INDEX NAME)

CH2

RN 849431-08-9 CAPLUS (1,4-piazabicyclo[3.2.2]nonane, 4-[[4-(3-bromophenyl)-2-thiazolyl]methyl]-(9c1) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

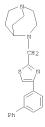
N CH2

RN 849431-09-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-phenyl-2-thiazolyl)methyl]- (9CI)
(CA INDEX NAME)

CH2 S N

RN 849431-10-3 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-[1,1'-biphenyl]-3-yl-2-thiazolyl)methyl]- (9CI) (CA INDEX NAME)

L15 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L15 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1997:701404 CAPLUS DOCUMENT NUMBER: 127:355342

TITLE: Aralkyl-bridged diazabicycloalkane derivatives for CNS

INVENTOR(S):

disorders, and preparation thereof Bowen, Wayne; De Costa, Brian R.; Dominguez, Celia; He, Xiao-Shu; Rice, Kenner C. United States Dept. of Health and Human Services, USA U.S., 13 pp., Cont. of U.S. Ser. No. 950,359, abandoned. CODEN: USXXAM PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND

DATE APPLICATION NO. DATE HS 5679673 А 19971021 US 1994-344304 19941121 PRIORITY APPLN. INFO.:

AB Certain aralkyl diazabicycloalkyl compds. are described for treatment of Certain aralkyl diazabicycloalkyl compds. are described for treatment of CNS disorders, e.g. cerebral ischemia, psychoses, and convulsions. Compds. of particular interest are I (R, Rl, R4, R5, R6, R7 = H, lower alkyl, benzyl, halo-lower alkyl, R2, R3, R10-R13 = H, OH, lower alkyl, benzyl and halo-lower alkyl; R2, R3, R10-R13 = H, OH, lower alkyl, benzyl and halo-lower alkyl; me = 2-4; A = Ph, naphthyl, benzothiophenyl, benzofuranyl, thienyl, wherein any of the foregoing A groups can be further substituted with 21 of H, OH, lower alkyl, lower alkoxy, halo, halo-lower alkyl, amino, mono- and di-lower alkylamino), or a pharmaceutically acceptable salt thereof. Preparation of 4-[2-(3,4-Dichlorophenyl)ethyl]-1,4-diazabicyclo[2.2.3] nonane is described, as is its activity in a sigma receptor assay.

RL: BAC (Biological activity or effector, except adverse); BPR (Biological

L15 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L15 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PRCC (Process); USES (Uses) (Preparation); PRC: (Process); USES (USES)
(aralkyl-bridged diazabicycloalkane derivs. for CNS disorders, and prepn. thereof)
150235-80-6 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-[2-(3,4-dichlorophenyl)ethyl]- (9CI)

INDEX NAME)

IT

198482-85-8 198482-87-0 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(Uses)

(aralkyl-bridged diazabicycloalkane derivs. for CNS disorders, and preparation thereof)
198482-85-8 CAPLUS
1,4-Diazabicyclo[3.2.2]nonane, 4-(2-benzo[b]thien-3-ylethyl)- (9CI) (CA

INDEX NAME)

198482-87-0 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-[2-(2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

L15 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1995:313069 CAPLUS

DOCUMENT NUMBER:

1995:31309 CAPLUS
122:12295
Cytotoxic effects of sigma ligands: sigma
receptor-mediated alterations in cellular morphology
and viability
Vilner, Bertold J.; de Costa, Brian R.; Bowen, Wayne

AUTHOR(S):

CORPORATE SOURCE:

D. Unit Receptor Biochem. Pharmacology, National Inst. Diabetes Digestive Kidney Diseases, Bethesda, MD,

CORPORATE SOURCE: Unit Receptor Biochem. Pharmacology, National Inst.
Diabetes Digestive Kidney Diseases, Bethesda, MD,
20892, USA

SOURCE: Journal of Neuroscience (1995), 15(1, Pt. 1), 117-34
CODEN: JNRSDS; ISSN: 0270-6474

PUBLISHER: Society for Neuroscience
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The morphol. effects of several neuroleptics as well as other novel and
prototypic sigma ligands were examined by addition to cultures of C6

na cells. Sigma ligands caused loss of processes, assumption of spherical shape, and cessation of cell division. The time course and magnitude of this effect were dependent on the concentration of sigma ligand.

Continued

exposure to sigma compds. ultimately resulted in cell death. However,

morphol. effect was reversible when sigma ligand was removed shortly after

rounding. The potency of compds. to produce these effects generally correlated with binding affinity at sigma receptors of C6 glioma cells membranes labeled with [3H](+)-pentazocine. At a concentration of 100

haloperidol, reduced haloperidol, fluphenazine, has a concentration of 100 haloperidol, reduced haloperidol, fluphenazine, perphenazine, BD737, LR172, BE1008, and SH344 produced significant effects in 3-6 h of exposure. Other compds., such as trifluoperidol, thloridazine, and (-)-butaclannol, produced significant effects by 24 h of exposure. Despite the requirement of micromolar concess. of ligand (some compds. were effective at 30 µm), the effect showed a remarkable specificity for compds. exhibiting sigma receptor binding affinity. Neuroleptics lacking potent sigma affinity [e.g., (-)-sulpride, (+)-butaclamol, and clozapinel and other compds. that lack significant sigma affinity but that are agonists or antagonists at dopamine, serotonin, adrenergic, glutamate, phencyclidine, GABA, opiate, or muscarinic cholinergic receptors were without effect on cellular morphol. at concess up to 300 µM over a period of 72 h. Likewise, blockers and activators of Na+, K+, and Ca2+ channels and a monoamine oxidase bitor

oltor devoid of sigma affinity were without effect. Interestingly, 1,3-di-o-tolylguanidine (UTG), (+)-3-(3-hydroxyphenyl)-N-(1-propyl)plperidine [(+)-3-PPP], (+)-pentazocine, (+)-cyclazocine, and

sigma-active benzomorphans and morphinans appeared inactive in up to 72 h of culture. However, these compds. interacted synergistically with a subeffective dose of BD737 (30 µM) to produce effects usually in 6 h or less. Also, the pH of the culture medium had a profound effect on the activity of sigma compds. Increasing the pH from the normal range of 7.2-7.4 to pH 8.3-8.5 shifted the dose curves (30, 100, 300 µM) for all sigma compds. to the left. Under these conditions, DTG, (+)-3-PPP, and benzomorphans produced effects in 24 h or less. Decreasing the medium pH to 6.5-6.7 markedly reduced the activity of all sigma ligands, producing

L15 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) significant protection from cytotoxic effects. Importantly, compds. that lacked sigma binding affinity showed neither synergism with 30 µM MD737 nor an increase in activity at higher pH. These results confirm the receptor specificity of this effect. Sigma ligands had similar effects on other cells of neuronal and non-neuronal origin, including SK-N-SH and SH-SY5Y neuroblastomas, NCB-20 hybridoma, NS 108-15 neuroblastoma-glioma hybrid, COS-7 (kidney), MRS-5 (lung), and FC12 pheochromosome vital role in cell function and may have important implications for neurodegenerative disorders and neuroleptic treatment.

IT 150235-80-6, BD 1216
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study) (cytotoxic effects of sigma ligands: sigma receptor-mediated alterations in cellular morphol. and viability)

RN 150235-80-6 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[2-(3,4-dichlorophenyl)ethyl]- (9CI) (CA

L15 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) dichlorophenyl)ethyl]-4-alkylpiperazines suggests that the 2 N atoms of I are working in opposition to one another in terms of their sensitivity to steric bulk. The high binding affinity of 1,4-diazabicylo[4,3.0]nonanes suggests that these may approx. the Me and pyrrolidine ring conformations found in I when it is bound to the or receptor. Binding data suggest that the conformation of I favors strong binding interaction at orreceptors. G-Receptor Ki's was 0.55 nM for 1-[2-(3,4-dichlorophenyl)ethyl]-4-n-butylpiperarine. Overall comparison of the results indicate that I is subject to considerable conformational freedom and suggests that the orreceptor is not subject to rigid stereochem. restraints with I. These results corroborate an earlier study

study

Where I was restrained using simple monocyclic heterocycles. 150235-81-7P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as o-receptor antagonist) 150235-81-7 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[2-(3,4-dichlorophenyl)ethyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CRN 150235-80-6 CMF C15 H20 C12 N2

CM 2

Double bond geometry as shown.

L15 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1994:106904 CAPLUS

DOCUMENT NUMBER: 120:106904

Synthesis and evaluation of conformationally TITLE:

TITLE: Synthesia and evaluation of the restricted  $N-[2-(3,4-dichloropheny1)] = N-methyl-2- \\ (1-pyrrolidiny1) = thylloropheny1) = thyllo$ 

AUTHOR(S).

and miscellaneous compounds de Costa, Brian R.; He, Xiaoshu; Linders, Joannes T. M.; Dominguez, Celia; Gu, Zi Qiang; Williams, Wanda; Bowen, Wayne Lab. Med. Chem., Natl. Inst. Diabetes Dig. Kidney Dis., Bethesda, MD, 20892, USA Journal of Medicinal Chemistry (1993), 36(16),

CORPORATE SOURCE:

CODEN: JMCMAR; ISSN: 0022-2623 Journal English CASREACT 120:106904

DOCUMENT TYPE: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

a continuation of an earlier study (J. Med. Chemical 1992, 35,

-4343) the  $\sigma$ -receptor ligand was conformationally restricted in 2-(1-pyrrolidiny1)-N-[2-(3,4-dichloropheny1)ethy1]-N-methylethylamine (I) by incorporating it into homologous piperazines and homopiperazines, diazabicyclononanes and decanes, bridgehead bicycloctanes and nonanes as well as other miscellaneous compds.  $\sigma$ -Receptor binding affinities were obtained using [3H] (+)-pentazorine in guinea pig brain membranes. Probably the N lone pair orientation found in the piperazines affords the strongest binding interaction. Other N lone pair orientations or compds. representing unlikely staggered conformations of I [as in 4-[2-(3,4-dichloropheny1)ethy1]-1,4-diazabicyclo[3.2.2]nonane] show very weak o interaction. Comparison of the binding data of different N-substituted homologs of I with those of the 1-[2-(3,4-

L15 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1991:102068 CAPLUS DOCUMENT NUMBER: 114:102068

US COPYRIGHT 2007 ACS on STN
1991:102068 CAPLUS
114:102068
1,4-diazabicyclo[3.2.2]nonane as a bactericide intermediate
readmann, Robert C.; Lackey, John W.
Pfizer Inc., USA
Can. Pat. Appl., 31 pp.
CODEN: CPXXEB
Patent
English
2

INVENTOR (S)

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
	CA 2001211	A1	19900425	CA 1989-2001211		19891023
	US 4895943	A	19900123	US 1988-262542		19881025
PRIOR	RITY APPLN. INFO.:			US 1988-262542 A	À.	19881025

MARPAT 114:102068 OTHER SOURCE(S):





AB Compds. [I; X = CO, CH2; R = H, (un)substituted benzyl, benzoyl, or naphthoyl; Q = H; W = CH2CH2OH, CH2CO2R1, CH2CH2R2; R1 = C1-4

naphthoyi, w · .., ..
(halo]alkyl;
R2 = leaving group; WQ can form CH2CH2, with provisos; and II; R ≠ H
= (un)substituted benzyl, benzoyl, naphthoyl] were prepared by

cyclization
 of dicarboxylate esters R102CCH2CH(NHCH2CH2NH2)CH2CO2R3 [III; R1, R3 =
 C1-4 (halo)alkyl] with an alkyl stannate or trialkylaluminum,
benzoylation
 of the resulting diazepinone (VI; R4 = benzoyl; R5 = CO2R1), reduction

of the product to a hydroxyethyldiazepine analog followed by OH-group activation and ring closure of the latter. Thus, refluxing III (R1 = R3 = Et) (preparation given) 18 h with (n-Bu)3Sn803GF3 followed by benzoylation gave 78%

IV (R4 = PhCO, R5 = CO2Et). This in THF was refluxed 18 h with LiAlH4, the product (100%) refluxed 1 h with SOCI2 and the chlorocthyl derivative (64%) stirred 1 h with 50% aqueous NaOH to give the title base II (R = H) which was converted to its ditosylate salt (51%). The free base was sufficiently pure to be used to prepare (preparation not given) bactericide binfloxacin.

IT 127783-88-4P

L15 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenolysis of)
RN 127783-88-4 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(phenylmethyl)- (9CI) (CA INDEX NAME)



L15 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1990:423956 CAPLUS DOCUMENT NUMBER: 113:23956 113:23950
Preparation of diazabicyclononanes as intermediates
for antibacterial quinolones
Friedmann, Robert C.; Lackey, John W.; O'Neill, Brian TITLE: INVENTOR(S): Pfizer Inc., USA PATENT ASSIGNEE(S): U.S., 6 pp. CODEN: USXXAM Patent DOCUMENT TYPE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4895943	Α	19900123	US 1988-262542	19881025
US 5026845	A	19910625	US 1989-417120	19891004
EP 366301	A2	19900502	EP 1989-310389	19891011
EP 366301	A3	19910731		
EP 366301	B1	19940831		
R: AT, BE, CH	, DE, ES	, FR, GB,	GR, IT, LI, LU, NL, SE	
IL 92025	A	19941007	IL 1989-92025	19891017
CA 2001211	A1	19900425	CA 1989-2001211	19891023
DK 8905269	A	19900426	DK 1989-5269	19891024
NO 8904230	A	19900426	NO 1989-4230	19891024
NO 172050	В	19930222		
NO 172050	C	19930602		
AU 8943700	A	19900503	AU 1989-43700	19891024
AU 616062	B2	19911017		
HU 54366	A2	19910228	HU 1989-5422	19891024
HU 205116	В	19920330		
ZA 8908047	A	19910626	ZA 1989-8047	19891024
JP 02174769	A	19900706	JP 1989-278301	19891025
JP 06099408	В	19941207		
PRIORITY APPLN. INFO.:			US 1988-262542	A3 19881025

OTHER SOURCE(S): CASREACT 113:23956; MARPAT 113:23956



AB Bicyclo compds. I [R2 = (substituted) naphthoyl, benzyl, benzoyl, etc.] were prepared Treatment of 4-phenylmethyl-5-(2-hydroxyethyl)-1,4-diazepine with SOCl2, ring closure, hydrogenolysis over Pd(OH)2, and treatment with toluenesulfonic acid, gave 1,4-diazabicyclo[3.2.2]nonane ditosylate salt.

L15 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 127783-88-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, in preparation of intermediate for quinolone olone
antibacterial)
127783-88-4 CAPLUS
1,4-Diazabicyclo[3.2.2]nonane, 4-(phenylmethyl)- (9CI) (CA INDEX NAME)



L15 ANSWER 9 OF 9
ACCESSION NUMBER:
DOCUMENT NUMBER:
1977:155489 CAPLUS
S6:155489 SAPLUS
Synthesis and pharmacological study of quinuclidine analogs of sulpiride and bithiodine
Mikhlina, E. E.; Vorob'eva, V. Ya.; Komarova, N. A.;
Sharapov, I. N.; Polezhaeva, A. I.; Mashkovskii, M. D.; Yakhontov, L. N.
CORPORATE SOURCE:

SOURCE:
Khimiko-Farmatsevticheskii Zhurnal (1976), 10(11),
56-60
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE:
JOURNAL
JOURN DOCUMENT TYPE: LANGUAGE: GI

R<sup>1</sup> I N(CH<sub>2</sub>)3NHR<sup>1</sup> II

(In this abstract R = 5-sulfamoyl-o-anisoyl). Reaction of quinuclidines I (RI = 2-CH2NH2, 3-XNH2, 4-NH2, X = bond, CH2CH2, CCH2CH2CH2) with ROEt gave 83.4-97% I (RI = 2-CH2NHR, 3-XNHR, 4-NHR). Similar treatment of II (RI = H) gave 97% II (RI = R) = bond, (CH2)3] were preparation similarly in 84-97% yield. Treatment of Et 3-quinuclidinecarboxylate

with

with
2-thienylmagnesium bromide gave 36.7%
3-quinuclidinyldi-2-thienylcarbinol,
which was dehydrated to give 69% methylene derivative None of the prepared

red compds. had antiemetic activity. LD50 were 9.3-415.0 mg/kg (i.v. white mice). In narcotized cats all prepared compds. at 3-10 mg/kg

compds. had antiemetic activity. LD50 were 9.3-415.0 mg/kg (1.v. white mice). In narcotized cate all prepared compds at 3-10 mg/kg simultaneously increased the arterial pressure. The quinuclidine derivs. did not have favorable antimetic properties when compared to bithiodine nor did they have significant activity on the cholino- and histaminergic systems.

IT 62190-19-6P

L15 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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NEWS 4 JUL 02 CHEMCATS accession numbers revised

NEWS 5 JUL 02 CA/CAplus enhanced with utility model patents from China

NEWS 6 JUL 16 CAplus enhanced with French and German abstracts

NEWS 7 JUL 18 CA/CAplus patent coverage enhanced

NEWS 8 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification

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NEWS 11 AUG 06 FSTA enhanced with new thesaurus edition

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NEWS 17 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index

NEWS 18 SEP 13 FORIS renamed to SOFIS

NEWS 19 SEP 13 INPADOCDB enhanced with monthly SDI frequency

NEWS 20 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998

NEWS 21 SEP 17 CAplus coverage extended to include traditional medicine patents

NEWS 22 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements

NEWS 23 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt

NEWS 24 OCT 19 BEILSTEIN updated with new compounds

NEWS 25 NOV 15 Derwent Indian patent publication number format enhanced

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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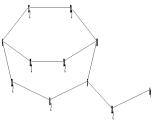
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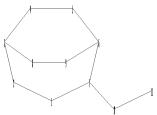
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http://www.cas.org/support/stngen/stndoc/properties.html

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chain nodes :

10 11

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds: 7-10 10-11 ring bonds:

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 6-9 8-9

exact/norm bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 6-9 8-9 10-11

exact bonds :

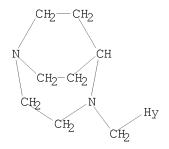
7-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

46 ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 10:38:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3834 TO ITERATE

52.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
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PROJECTED ITERATIONS: 72967 TO 80393 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 10:38:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 77369 TO ITERATE

100.0% PROCESSED 77369 ITERATIONS SEARCH TIME: 00.00.04

L3 46 SEA SSS FUL L1

=> d scan

46 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(2-pyridiny1)-2-thieny1]methy1]-C17 H21 N3 S

46 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-chlorophenyl)-2-thienyl]methyl]-C18 H21 C1 N2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

46 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-thiazolylmethyl)-C11 H17 N3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 46 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Formic acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-6methoxy-4H-1-benzopyran-4-one (1:1)
MF C18 H22 N2 03 . C H2 02 CM 1

О=СН−ОН

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=>

=> s 13

L4 2 L3

=> d 14 1-2 ibib abs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:1241229 CAPLUS 2003:1241229 CAPLUS
144:6818
Indazoles, benzothiazoles, 1,2-benzoisoxazoles,
1,2-benzoisothiazoles, and chromones as a7
nicotinic receptor agonists, their preparation,
pharmaceutical compositions, and use in therapy
Xie, Wenge; Herbert, Brian; Schumacher, Richard A.;
Ma, Jianquo; Ngupen, Truc Minh; Gauss, Carla Maria;
Tehim, Ashok
Memory Pharmaceuticals Corporation, USA
PCT Int. Appl., 143 pp.
CODEN: PIXXD2
Patent
English
1 DOCUMENT NUMBER: TITLE: INVENTOR(S): PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.					KIND DATE													
					A2	A2 20051124												
	2005				A3		2006	0831										
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	KZ,	
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	
							PH,											
		SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	
		ZM,																
	RW:						MW,											
							RU,											
							GR,											
							BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	
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AU	U 2005243147				A1		2005	1124	AU 2005-243147						20050506 20050506			
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EP	1745													on		0050		
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						LU,	MC,	NL,	PL,	PT,	KO,	SE,	SI,	SK,	TK,	AL,	BA,	
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	2006						2007	0031	IN 2006-DN6854 NO 2006-5622						20061117			
TAD	2006	2156	07		7.											0061		
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										US 2	004-	5747	12P	1	P 2	0040	527	
										US 2	004-	5264	59P	1	P 2	0041	110	
										WO 2	005-1	JS15:	937	1	W 2	0050	506	

(Uses)
(drug candidate; preparation of heteroaryl-substituted
diazabicyclo[3.2.2]nonanes as α7 nicotinic receptor agonists)
RN 869783-40-4 CAPLUS
CN 4H-1-Benzopyran-4-one,
3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-6-methoxy(CA INDEX NAME)

869783-41-5 CAPLUS Formic acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-6-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CM 1

CRN 869783-40-4 CMF C18 H22 N2 O3

CRN 64-18-6

Page 29

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): CASREACT 144:6818; MARPAT 144:6818

The invention relates to heteroaryl-substituted azabicyclic compds.,

I or II, which are ligands for nicotinic acetylcholine receptors (nAChR) and can be used for the activation of nAChRs and the treatment of disease conditions associated with defective or malfunctioning nicotinic acetylcholine receptors, especially of the brain. In compds. I and II,

CH2, C=0, or C=S; m is 1 or 2; Y is 0 or S; X1 to X4 are independently selected from N and (un)substituted C, wherein at most one of X1 to X4 is N; X5 and X6 are independently selected from CH, fluoro-substituted Cl-6 alkoxy-C, and heterocyclyl-C, wherein no more than one of X5 and X6 is CH:

X7 is CH or N; and R is H, (halo)-C1-4 alkyl, C3-7 cycloalkyl, C4-7 cycloalkylalkyl, and C1-6 alkyl-C6-10 aryl. The invention also relates

the preparation of the heteroaryl-substituted diazabicyclic compds., pharmaceutical compns. comprising those compds. and a pharmaceutically acceptable carrier, as well as to the use of the compns. as agonists for the  $\alpha 7$  nAchR subtype. Acylation of 3-methoxythiophenol with oxalyl

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN CMF C H2 O2 (Continued)

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RN 869783-44-8 CAPLUS CN 4H-1-Benzopyran-4-one, 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-5-methoxy-(CA INDEX NAME)

869783-45-9 CAPLUS Formic acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-5-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CM 1

CRN 869783-44-8 CMF C18 H22 N2 O3

CM 2

CRN 64-18-6 CMF C H2 O2

о≕сн−он

RN 869783-48-2 CAPLUS CN 4H-1-Benzopyran-4-one, 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-7-methoxy-(CA INDEX NAME)

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

869783-49-3 CAPLUS Despise acid, compd. with 3-(1,4-diazabicyclo[3.2.2]non-4-ylmethyl)-7-methoxy-4H-1-benzopyran-4-one (1:1) (CA INDEX NAME)

CRN 869783-48-2 CMF C18 H22 N2 O3

CM

CRN 64-18-6 C H2 O2

о=сн−он

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) thiazolyl, oxazolyl, or imidazolyl, etc.; D is H, alkyl, Ph, or pyridyl, etc.], useful as nicotinic acetylcholine agonists. For instance, diazabicyclononane deriv. I was prepd. via reductive amination of phenylpropargyl aldehyde by 1,4-diazabicyclo[3.2.2]nonane dihydrochloride.

Biol. investigation included assays for detg. affinity at α7 nAChR and α4 nAChR (Ki values were less than 1000 nM in both tests).

IT 849430-68-8Pp, (1,4-Diazabicyclo[3.2.2]non-4-yl)(6-bromopyridin-2-yl)methane

RL: PAC (Pharmacological activity); RCT (Reactant); SFN (Synthetic preparation); THU (Therapeutic use); BTOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of diazabicyclononane derivs. useful as nicotinic acetylcholine

agonists)

RN 849430-68-8 CAPLUS

CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(6-bromo-2-pyridinyl)methyl]- (CA INDEX)

NAME)

849430-60-0P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (5-phenylfuran-2-yl)methane 849430-62-2P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (5-phenylfuran-2-yl)methane 849430-62-2P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (5-phenylfuhlophen-2-yl)methane 849430-63-3P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (benzofuran-2-yl)methane 849430-66-6P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (quinolin-3-yl)methane 849430-70-2P, (1,4-Diazabicyclo[3.2.2]non-4-yl) (quinolin-3-yl)methane 849430-71-3P, 4-(4-Phenylfuhlophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-72-4P, 4-[5-(Pyridin-2-yl)methyl)-1,4-diazabicyclo[3.2.2]nonane 849430-73-6-8P, 4-(6-Phenylpyridin-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-76-8P, 4-(6-Phenylpyridin-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-83-7P, (1,4-Diazabicyclo[3.2.2]non4-yl)[5-(3-pyridyl)thiophen-2-yl]methane 849430-85-9P, (1,4-Diazabicyclo[3.2.2]non4-yl)[5-(4-pyridyl)thiophen-2-yl]methane 849430-85-9P, (1,4-Diazabicyclo[3.2.2]non4-yl)[4-(3-pyridyl)thiophen-2-yl]methane 849430-85-9P, (1,4-Diazabicyclo[3.2.2]non4-yl)[4-(3-pyridyl)thiophen-2-yl]methane 849430-85-9P, (1,4-Diazabicyclo[3.2.2]non4-yl)(14-(3-pyridyl)thiophen-2-yl]methane 849430-85-9P, (1,4-Diazabicyclo[3.2.2]non4-yl)(14-(3-pyrid

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:300453 CAPLUS DOCUMENT NUMBER: 142:373869

TITLE:

142:773869
A preparation of diazabicyclononane derivatives,
useful as nicotinic acetylcholine agonists
Ernst, Glen; Phillips, Elfion; Schmiesing, Richard J.
Astrazeneca AB, Swed.; Astrazeneca UK Ltd.
PCT Int. Appl., 34 pp.
CODEN: FIXXD2 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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	US 2007043031				A1		2007	0222		US 2	006-	5731	32		20061023					
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WO 2004-GB4130

W 20040924

CASREACT 142:373869; MARPAT 142:373869 OTHER SOURCE(S):

The invention relates to a preparation of diazabicyclononane derivs. of

Q-E-D [wherein: Q is diazabicyclononane derivative; E is alk(en/yn)yl,

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) yl)methane 849430-89-3P, (1,4-Diazabicyclo[3.2.2]non-4-yl)(4-phenylpyridin-2-yl)methane 849430-90-6P, (1,4-piazabicyclo[3.2.2]non-4-yl)(5-phenylpyridin-2-yl)methane 849430-90-6P, (1,4-piazabicyclo[3.2.2]non-4-yl)(5-phenylpyridin-2-yl)methane 849430-90-7P, 4-(4-Enscomthiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-92-8P, 4-(5-Bromothiophen-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849430-93-9P, 4-[4-(4-Methoxyphenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-93-PP, 4-[4-(4-Chlorophenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-95-1P, 4-[5-(4-Methoxyphenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-95-1P, 4-[5-(4-Methoxyphenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-97-3P, 4-[5-(3-Chlorophenyl)thiophen-2-ylmethyl]-1,4-diazabicyclo[3.2.2]nonane 849430-99-5P, 4-[5-(4-Phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-5-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(2-Phenylthiazol-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(4-Methyl)-Benzinidazol-2-ylmethyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(4-Methyl)-1,4-diazabicyclo[3.2.2]nonane 849431-03-4P, 4-(4-M anazabicycio[.2.2]monane 649431-10-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diazabicyclononane derivs. useful as nicotinic acetylcholine
agonists)
RN 849430-60-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-furanyl)methyl]- (CA INDEX

NAME)

849430-62-2 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-thienyl)methyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

849430-63-3 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-benzofuranylmethyl)- (CA INDEX NAME)

849430-66-6 CAPLUS 1,4-Dlazabicyclo[3.2.2]nonane, 4-(benzo[b]thien-3-ylmethyl)- (CA INDEX NAME)

849430-69-9 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(3-quinolinylmethyl)- (CA INDEX NAME)

849430-70-2 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-quinolinylmethyl)- (CA INDEX NAME)

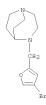
- ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 849430-74-6 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-pyridinylmethyl)- (CA INDEX NAME)



849430-76-8 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(6-phenyl-2-pyridinyl)methyl]- (CA INDEX NAME)



849430-79-1 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-bromo-2-furanyl)methyl]- (CA INDEX NAME)



Page 31

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

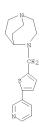
849430-71-3 CAPLUS

1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-phenyl-2-thienyl)methyl]- (CA INDEX NAME)

849430-72-4 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(2-pyridinyl)-2-thienyl]methyl]-

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 849430-83-7 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(3-pyridinyl)-2-thienyl]methyl]-

INDEX NAME)



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INDEX NAME)

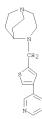


849430-85-9 CAPLUS 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(2-pyridinyl)-2-thienyl]methyl]-

INDEX NAME)

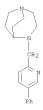
L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 849430-86-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(3-pyridinyl)-2-thienyl]methyl](CA TUNEY NAME)



RN 849430-87-1 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-pyridinyl)-2-thienyl]methyl](CA
TNDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) INDEX NAME)



RN 849430-91-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-bromo-2-thienyl)methyl]- (CA INDEX NAME)

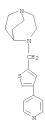


RN 849430-92-8 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-bromo-2-thienyl)methyl]- (CA INDEX NAME)



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L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



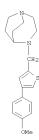
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CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(3-isoquinolinylmethyl)- (CA INDEX NAME)

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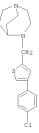
RN 849430-90-6 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(5-phenyl-2-pyridinyl)methyl]- (CA

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 849430-93-9 CAPLUS
CN 1,4-Diazabicyclo(3.2.2]nonane, 4-[[4-(4-methoxypheny1)-2-thieny1]methy1](CA INDEX NAME)



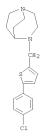
RN 849430-94-0 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(4-chloropheny1)-2-thieny1]methy1]-(CA INDEX NAME)



RN 849430-95-1 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(4-methoxyphenyl)-2-thienyl]methyl](CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 849430-96-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(4-chlorophenyl)-2-thienyl]methyl](CA INDEX NAME)



RN 849430-97-3 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[[5-(3-chloropheny1)-2-thieny1]methy1]-(CA INDEX NAME)

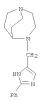
L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(5-thiazolylmethyl)- (CA INDEX NAME)



RN 849431-01-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-5-thiazolyl)methyl]- (CA INDEX NAME)



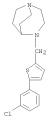
RN 849431-02-3 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-1H-imidazol-4-y1)methyl](9C1) (CA INDEX NAME)



RN 849431-03-4 CAPLUS

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L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 849430-98-4 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-quinoxalinylmethyl)- (CA INDEX NAME)

RN 849430-99-5 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-bromo-5-thiazoly1)methy1]- (CA INDEX NAME)



RN 849431-00-1 CAPLUS

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-thiazolylmethyl)- (CA INDEX NAME)



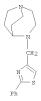
RN 849431-04-5 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-(2-benzothiazolylmethyl)- (CA INDEX NAME)

RN 849431-05-6 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(1-methyl-1H-benzimidazol-2-yl)methyl]-(CA INDEX NAME)

RN 849431-06-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(3-methyl-5-phenyl-2-thienyl)methyl](CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 849431-07-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(2-phenyl-4-thiazoly1)methyl]- (CA INDEX NAME)

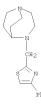


RN 849431-08-9 CAPLUS (1,4-Diazabicyclo[3.2.2]nonane, 4-[[4-(3-bromophenyl)-2-thiazolyl]methyl]-(CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

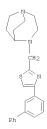


RN 849431-09-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-phenyl-2-thiazoly1)methyl]- (CA INDEX NAME)



RN 849431-10-3 CAPLUS CN 1,4-Diazabicyclo[3.2.2]nonane, 4-[(4-[1,1'-biphenyl]-3-yl-2-thiazolyl)methyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

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---Logging off of STN---

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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	22.76	195.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

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